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THE FREE ENERGY OF THE SPIN-BOSON MODEL

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Abstract : For n spins $\frac{1}{2}$ coupled linearly to a boson field in a volume V_n, the existence of the specific free energy in the limit $n \to \infty$, $V_n \to \infty$ with n/V_n = const., is proved under specified conditions on the Hamiltonian. A variational expression is obtained for the limiting specific free energy, and a critical temperature is identified, above which the system behaves as if there were no coupling at all.

§1. Introduction, and main result

Consider the Hamiltonian

$$H_n = \sum_{\nu\geq 1} \omega_n(\nu) a^*_\nu a_\nu + V_n^{-\frac{1}{2}} \sum_{\nu\geq 1} \sum_{j=1}^{n} \{\lambda_n(j;\nu) a^*_\nu + \overline{\lambda_n(j;\nu)} a_\nu\} S^x_{(j)}$$

$$+ \sum_{j=1}^{n} \varepsilon_n(j) S^z_{(j)} \quad ,$$

for n spins $\frac{1}{2}$ - described by the spin operators $\{S^\alpha_{(j)} : j=1,2,\cdots,n; \alpha=x,y,z\}$, with $[S^x_{(j)}, S^y_{(k)}] = i\delta_{jk} S^z_{(j)}$ and cyclic permutations - interacting linearly with a countable number of bosonic degrees of freedom described by creation/annihilation operators $\{a^*_\nu, a_\nu : \nu\geq 1\}$, with $[a_\nu, a^*_{\nu'}] \subset \delta_{\nu,\nu'}$. The *strictly positive* bosonic frequencies $\omega_n(\nu)$ are assumed to satisfy

$$\sum_{\nu\geq 1} e^{-\beta\omega_n(\nu)} < \infty \quad , \text{ for } \beta > 0 \ ;$$

the coupling constants $\{\lambda_n(j;\nu) : \nu\geq 1, \ j=1,2,\cdots,n\}$ are complex numbers satisfying

$$\sum_{\nu\geq 1} |\lambda_n(j;\nu)|^2 < \infty \quad , \text{ for every } j=1,2,,\cdots,n \ ;$$

and the $\{\varepsilon_n(j) : j=1,2,\cdots,n\}$ are real.

The problem is to determine the specific free energy of the system in the thermodynamic limit $n \to \infty$, where V_n - the volume of the system - is proportional to n, that is to say $\rho=n/V_n$ - the density of the spins - is constant. This problem has been solved in a number of particular cases. Firstly, Hepp and Lieb [8], treated the case of 1 bosonic mode using a rotating-wave approximation for the coupling (Dicke Maser Model). These same authors then [9] removed the latter approximation and treated finitely many bosonic modes in the *homogeneous* case where the coupling constants and spin frequencies are independent of the spins: $\lambda_n(j;\nu)=\lambda_n(\nu)$, and $\varepsilon_n(j)=\varepsilon_n$ for every $j=1,2,\cdots,n$. Hepp and

Lieb , also obtain results on thermodynamic stability for the general (i.e. *heterogeneous*) model, leaving open the question of existence of the thermodynamic limit (9). Subsequently, the "Approximating Hamiltonian Method" has been put to work on the Hamiltonian H_n and its variants (2,3,12). The homogeneous case with countably many bosonic modes has been treated in detail (10) using large deviation methods developed in ref. 4.

Here, the problem is solved for the heterogeneous model using a method developed by Duffield and Pulè in their treatment of the B.C.S. model (6), supplemented with an idea of Bogoljubov (jr.) and Plechko (3). It is shown that under certain specified conditions H_n is thermodynamically equivalent (in the sense that the difference of the specific free-energies vanishes in the thermodynamic limit) to the Hamiltonian

$$\tilde{H}_n = \sum_{\nu\geq 1} \omega_n(\nu) a^*_\nu a_\nu + \sum_{j=1}^{n} \epsilon_n(j) S^z_{(j)} - V_n^{-1} \sum_{j,k=1}^{n} \Lambda_n(j,k) S^x_{(j)} S^x_{(k)} \quad ,$$

where the spin-boson interaction is replaced by an effective quadratic spin-spin interaction:

$$\Lambda_n(j,k) = \mathrm{Re} \sum_{\nu\geq 1} \omega_n(\nu)^{-1} \overline{\lambda_n(j;\nu)} \lambda_n(k;\nu) \quad , \; j,k = 1,2,\cdots,n \; .$$

Moreover, $\tilde{H}_n$ is thermodynamically equivalent to the Hamiltonian

$$\hat{H}_n(x) = \sum_{\nu\geq 1} \omega_n(\nu) a^*_\nu a_\nu + \sum_{j=1}^{n} \epsilon_n(j) S^z_{(j)} + \sum_{j,k=1}^{n} \Lambda_n(j,k) x_j (V_n x_k 1 - 2S^x_{(k)}) \quad ,$$

if the real n-vector x is chosen so as to minimize the corresponding specific free energy.

The result is then the following:

<u>**Theorem**</u> <u>1</u>: *Suppose there exists real-valued continous functions* ε *on* $[0,1]$, *and* Λ *on* $[0,1]\times[0,1]$, *such that*

$$\lim_{n\to\infty} \sup_{j\in\{1,2,\cdots,n\}} |\epsilon_n(j) - \varepsilon(j/n)| = 0 \quad , \qquad \text{(C1)}$$

$$\lim_{n\to\infty} \sup_{j,k\in\{1,2,\cdots,n\}} |\Lambda_n(j,k)-\Lambda(j/n,k/n)|=0 \quad ; \tag{C2}$$

if

$$f^o = \lim_{\substack{n\to\infty \\ \rho=\text{const.}}} (-\beta V_n)^{-1} \log \operatorname{tr} \exp\{-\beta \sum_{\nu\ge1} \omega_n(\nu) a_\nu^* a_\nu\} \quad , \tag{C3}$$

exists for some $\beta > 0$, *and if*

$$\lim_{n\to\infty} n^{-3/2} \sum_{\nu\ge1} \omega_n(\nu)^{-\frac{1}{2}} \sum_{j=1}^{n} |\lambda_n(j;\nu)| = 0 \ , \tag{C4}$$

then

$$\lim_{\substack{n\to\infty \\ \rho=\text{const.}}} (-\beta V_n)^{-1} \log \operatorname{tr} \exp\{-\beta H_n\} = f^o - \rho \sup_{\substack{r,s\in L_{\mathbb{R}}^{\infty}([0,1]) \\ |s| \le r \le 1}} \left\{ \int_0^1 \left[\beta^{-1} I(r(t)) + \tfrac{1}{2}|\varepsilon(t)|[r(t)^2-s(t)^2]^{\frac{1}{2}}\right] dt + \tfrac{1}{4}\rho \int_0^1 \int_0^1 \Lambda(t,u)s(t)s(u)\,dt\,du \right\} \ ,$$

where $I(x) = -\frac{1}{2}(1+x)\log[\frac{1}{2}(1+x)] - \frac{1}{2}(1-x)\log[\frac{1}{2}(1-x)]$ for $0 \le x \le 1$.

This is proved in §3, after introducing notation in the following section 2. The solution of the variational problem, following Duffield and Pulè [6], is presented and briefly discussed in §4.

§2. Notation, definitions

It will be convenient to use Fock-space notation. For each $n=1,2,3...$, let $\mathcal{A}_n$ be a bounded region in $\mathbb{R}^d$ of volume (i.e. Lebesgue measure) V_n. Let $\mathfrak{h}_n$ be a positive *injective* selfadjoint operator on $L^2(\mathcal{A}_n)$ such that $\exp(-\beta\mathfrak{h}_n)$ is trace-class for $\beta > 0$. It follows that $\mathfrak{h}_n$ has a bounded inverse. Write $\mathfrak{K}_n$ for the n-fold tensor product of $\mathbb{C}^2$ and let $\underline{S}_{(j)}$ be a copy of of the Spin operator of magnitude $\frac{1}{2}$ acting on the j-th component of $\mathfrak{K}_n$ ($j=1,2,\ldots,n$). Let $\mathfrak{F}_n$ be the symmetric Fock space over $L^2(\mathcal{A}_n)$ and consider the Hamiltonian [1]

$$H_n = d\Gamma(\mathfrak{h}_n) + \sum_{j=1}^{n}\left\{(V_n)^{-\frac{1}{2}}(a^*(\lambda_n(j))+a(\lambda_n(j)))S^x_{(j)}+\varepsilon_n(j)S^z_{(j)}\right\} \quad (2.1)$$

acting on $\mathfrak{F}_n\otimes\mathfrak{K}_n$, where $\{\varepsilon_n(j)\}\subset\mathbb{R}$, $\{\lambda_n(j)\}\subset L^2(\mathcal{A}_n)$, $a(\cdot)$ is the familiar annihilation operator, and $d\Gamma$ denotes the second-quantization map. The quadratures formula (see ref. 5)

$$W[f]^*d\Gamma(\mathfrak{h})W[f] = d\Gamma(\mathfrak{h}) + a^*(\mathfrak{h}f)+a(\mathfrak{h}f) + \langle f,\mathfrak{h}f\rangle\cdot 1 , \quad (2.2)$$

valid for $f \in \mathrm{Dom}(\mathfrak{h})$ where $W[f]\equiv\exp\{\overline{a^*(f)-a(f)}\}$ is the unitary Weyl operator, enables one to write

$$H_n=\sum_{j=1}^{n}\left\{n^{-1}U_n(j)^*d\Gamma(\mathfrak{h}_n)U_n(j) + \varepsilon_n(j)S^z_{(j)} - \tfrac{1}{4}\rho\|\mathfrak{h}_n^{-\frac{1}{2}}\lambda_n(j)\|^2 1\right\} , \quad (2.3)$$

where the unitaries $U_n(j)$, $j=1,2,\cdots,n$, are given by

$$U_n(j) := W[\tfrac{1}{2}n(V_n)^{-\frac{1}{2}}\mathfrak{h}_n^{-1}\lambda_n(j)]P^+_{(j)}+ W[\tfrac{1}{2}n(V_n)^{-\frac{1}{2}}\mathfrak{h}_n^{-1}\lambda_n(j)]^*P^-_{(j)}, \quad (2.4)$$

where $P^\pm_{(j)}$ is the spectral projection of $S^x_{(j)}$ to the eigenvalue $\pm\frac{1}{2}$. Formula (2.3) can now be used to prove the self-adjointness of H_n.

Two free energy densities are associated with H_n:

$$\exp\{-\beta V_n f_n\} = \mathrm{tr}_{\mathfrak{F}_n\otimes\mathfrak{K}_n}(\exp\{-\beta H_n\}) , \quad (2.5)$$

$$\exp\{-\beta V_n f^o_n\} = \mathrm{tr}_{\mathfrak{F}_n}(\exp\{-\beta d\Gamma(\mathfrak{h}_n)\}) . \quad (2.6)$$

Of interest is the limit $n\to\infty$, such that V_n diverges but

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[1] Tensor notation for operators is not used, i.e. $S_{(j)}=1\otimes S_{(j)}$, $a(\circ)=a(\circ)\otimes 1$ etc.

$\rho=n/V_n$, remains *constant*.

The Hamiltonian (2.1) has the following symmetry. Let the self-adjoint, unitary operator L_n on $\mathfrak{F}_n \otimes \mathfrak{K}_n$ be given by $L_n = \Gamma(-1)(\prod_{j=1}^{n} 2S^z_{(j)})$; then $L_n S^z_{(j)} L_n = S^z_{(j)}$, and $L_n S^x_{(j)} L_n = -S^x_{(j)}$ for every $j=1,2,\cdots,n$, and $L_n d\Gamma(\circ) L_n = d\Gamma(\circ)$, $L_n a(\circ) L_n = -a(\circ)$. In particular, L_n commutes with H_n.

Consider the Hamiltonian $H_n(h)$, $h \in \mathbb{R}^n$, defined by

$$H_n(h) = H_n + \sum_{j=1}^{n} h_j S^x_{(j)} \quad , \tag{2.7}$$

where the symmetry of H_n implemented by L_n is *broken* if the external field vector h is non zero. The free energy density associated with $H_n(h)$ is written $f_n(h)$, and is a concave function of each of the n components of h. Expectation values with respect to the canonical state associated with $H_n(h)$ are denoted by $\langle\circ\rangle_h$.

The $(n\times n)$-matrix Λ_n is defined by its matrix elements

$$\Lambda_n(j,k) \equiv \mathrm{Re}\langle\lambda_n(j), \mathfrak{h}_n^{-1}\lambda_n(k)\rangle_{L^2(\mathcal{A}_n)} \quad , \quad j,k \in \{1,2,\cdots,n\} \quad ; \tag{2.8}$$

it is readily seen that Λ_n is *positive semi-definite* and the multiplicity of the eigenvalue 0 is equal to n minus the number of vectors in $\{\lambda_n(j): j=1,2,\cdots,n\}$ which are real-linearly independent.

§3. The proofs

Introduce a bosonic Hamiltonian $H^b_n(x)$, $x \in \mathbb{R}^n$, on $\mathfrak{F}_n$ by

$$H^b_n(x) = d\Gamma(\mathfrak{h}_n) + V_n \sum_{j=1}^{n} x_j \Big\{ V_n^{-\frac{1}{2}}(a^*(\lambda_n(j)) + a(\lambda_n(j))) + \sum_{k=1}^{n} \Lambda_n(j,k) x_k 1 \Big\} \quad , \tag{3.1}$$

and two spin Hamiltonians $\tilde{H}^s_n(h)$ and $\hat{H}^s_n(h;x)$, $h,x \in \mathbb{R}^n$, on $\mathfrak{R}_n$ by

$$\tilde{H}^s_n(h) = \sum_{j=1}^{n} \left\{ \epsilon_n(j) S^z_{(j)} + h_j S^x_{(j)} - V_n^{-1} \sum_{k=1}^{n} \Lambda_n(j,k) S^x_{(j)} S^x_{(k)} \right\}, \qquad (3.2)$$

$$\hat{H}^s_n(h;x) = \sum_{j=1}^{n} \left\{ \epsilon_n(j) S^z_{(j)} + \left\{ h_j - 2\sum_{k=1}^{n} \Lambda_n(j,k) x_k \right\} S^x_{(j)} \right\} + V_n x\Lambda_n x 1. \qquad (3.3)$$

Write $\tilde{f}^s_n(h)$, and $\hat{f}^s_n(h;x)$ for the free energy densities associated with (3.2) and (3.3) respectively. Expectation values with respect to a canonical state will be written as angular brackets indexed by the corresponding Hamiltonian or distinctive parameters characterizing it.

__Lemma 1__ :

$$(-\beta V_n)^{-1} \log \operatorname{tr}_{\mathfrak{Z}_n} \exp\{-\beta H^b_n(x)\} = f^o_n \ , \text{ for every } x \in \mathbb{R}^n \quad ;$$

$$\hat{f}^s_n(h;x) = x\Lambda_n x$$

$$- (V_n\beta)^{-1} \sum_{j=1}^{n} \log\left\{ 2\cosh\left\{ \tfrac{1}{2}\beta \left[\epsilon_n(j)^2 + (h_j - 2\sum_{k=1}^{n} \Lambda_n(j,k) x_k)^2 \right]^{\frac{1}{2}} \right\} \right\} .$$

__Proof__: An application of (2.2) shows that (3.1) is unitarily equivalent to $d\Gamma(\mathfrak{h}_n)$ for every $x \in \mathbb{R}^n$ (see the proof of Lemma 2A). Up to the constant term $V_n x\Lambda_n x 1$, the Hamiltonian (3.3) is the sum of n pairwise commuting operators

$$\epsilon_n(j) S^z + (h_j - 2\sum_{k=1}^{n} \Lambda_n(j,k) x_k) S^x \quad ,$$

on $\mathbb{C}^2$, each of which has $\pm\frac{1}{2}[\epsilon_n(j)^2 + (h_j - 2\sum_{k=1}^{n} \Lambda_n(j,k) x_k)^2]^{\frac{1}{2}}$ as its eigenvalues.■

Lemma 2A : $\tilde{f}^s_n(h) - \inf_{x\in\mathbb{R}^n} \hat{f}^s_n(h;x) \le f^o_n + \tilde{f}^s_n(h) - f_n(h)$.

Proof: Equivalently,

$$f^o_n + \inf_{x\in\mathbb{R}^n} \hat{f}^s_n(h;x) - f_n(h) \ge 0 \quad . \tag{*}$$

By the first part of Lemma 1, $f^o_n+\hat{f}^s_n(h;x)$ is the specific free energy associated with the Hamiltonian $\hat{H}_n(h;x) = H^b_n(x) + \hat{H}^s_n(h;x)$; by Bogoljubov's inequality (see ref. 7 for a proof)

$$f^o_n + \hat{f}^s_n(h;x) - f_n(h) \ge V_n^{-1}\langle \hat{H}_n(h;x)-H_n(h)\rangle_{\hat{H}_n(h;x)} \quad . \tag{**}$$

Now by (3.1),(3.2) and (2.7), the right-hand side of (**) is given by

$$\sum_{j=1}^{n}\left\{\left[V_n^{-\frac{1}{2}}\langle a^*(\lambda_n(j))+a(\lambda_n(j))\rangle_{H^b_n(x)} + 2\sum_{k=1}^{n}\Lambda_n(j,k)x_k\right]\right.$$

$$\left.\times\left[x_j - V_n^{-1}\langle S^x_{(j)}\rangle_{\hat{H}^s_n(h;x)}\right]\right\} \quad .$$

By (2.2), $H^b_n(x)=W[-V_n^{\frac{1}{2}}\sum_{j=1}^{n}x_j\mathfrak{h}_n^{-1}\lambda_n(j)]d\Gamma(\mathfrak{h}_n)W[V_n^{\frac{1}{2}}\sum_{j=1}^{n}x_j\mathfrak{h}_n^{-1}\lambda_n(j)]$. Using the formula $W[f]^*a(g)W[f]=a(g)+\langle g,f\rangle 1$ and (2.8),

$$\langle a^*(\lambda_n(k))+a(\lambda_n(k))\rangle_{H^b_n(x)} = \langle W[V_n^{\frac{1}{2}}\sum_{j=1}x_j\mathfrak{h}_n^{-1}\lambda_n(j)]$$

$$\cdot\{a^*(\lambda_n(k))+a(\lambda_n(k))\}W[-V_n^{\frac{1}{2}}\sum_{j=1}x_j\mathfrak{h}_n^{-1}\lambda_n(j)]\rangle_{d\Gamma(\mathfrak{h}_n)}$$

$$= -V_n^{\frac{1}{2}}\sum_{j=1}^{n}x_j\left[\overline{\langle\lambda_n(k),\mathfrak{h}_n^{-1}\lambda_n(j)\rangle} + \langle\lambda_n(k),\mathfrak{h}_n^{-1}\lambda_n(j)\rangle\right]$$

$$+ \langle a^*(\lambda_n(k))+a(\lambda_n(k))\rangle_{d\Gamma(\mathfrak{h}_n)} = -2V_n^{\frac{1}{2}}\sum_{j=1}^{n}\Lambda_n(j,k)x_j \quad .$$

Thus, the right-hand side of (**) is zero for every $x\in\mathbb{R}^n$; (*) follows by taking the infimum with respect to x.■

Bogoljubov's inequality also gives an upper bound on $f_n^o+\tilde{f}_n^s(h)-f_n(h)$; this involves

$$V_n^{-3/2}\sum_{\nu\geq 1}\sum_{j=1}^{n}\langle\{\lambda_n(j;\nu)a_\nu^* + \overline{\lambda_n(j;\nu)}a_\nu\}S^x_{(j)}\rangle_h \quad . \tag{3.4}$$

Bogoljubov and Plechko [3] have devised an alternative method which avoids the problem of estimating (3.4). Fix an arbitrary n, and consider an arbitrary finite number N of boson modes with strictly positive frequencies $\{\omega_n(\nu):1\leq\nu\leq N\}$, and associated coupling constants $\{\lambda_n(j;\nu):1\leq\nu\leq N,\ j=1,2,\cdots,n\}$. The Hamiltonian $H_n(h;N)$ is that obtained from $H_n(h)$ by considering only these N modes, and the associated specific free energy will be written $f_n(h;N)$; accordingly, write $f_n^o(N)$, and $\tilde{f}_n^s(h;N)$.

Let $\mathbb{A}=\{\nu:1\leq\nu\leq N,\ \lambda_n(j;\nu)=0$ for every $j=1,2,\cdots,n\}$, and $\mathbb{B}=\{1,2,\cdots,N\}\setminus\mathbb{A}$. For any set $\tau=\{\tau_\nu:\nu\in\mathbb{B}\}$ of real numbers in the open interval (0,1), one has the identity

$$H_n(h;N) = \sum_{\nu\in\mathbb{A}}\omega_n(\nu)a_\nu^*a_\nu + \sum_{\nu\in\mathbb{B}}(1-\tau_\nu)\omega_n(\nu)a_\nu^*a_\nu + \tilde{H}_n^s(h;N;\tau)$$

$$+ \sum_{\nu\in\mathbb{B}}\tau_\nu\omega_n(\nu)b_\nu(\tau)^*b_\nu(\tau) \quad , \tag{3.5}$$

where

$$\tilde{H}_n^s(h;N;\tau)=\sum_{j=1}^{n}\left\{\varepsilon_n(j)S^z_{(j)}+h_jS^x_{(j)}-V_n^{-1}\sum_{k=1}^{n}\Lambda_n^N(j,k;\tau)S^x_{(j)}S^x_{(k)}\right\} \quad , \tag{3.6}$$

$$\Lambda_n^N(j,k;\tau) = \mathrm{Re}\sum_{\nu\in\mathbb{B}}(\tau_\nu\omega_n(\nu))^{-1}\overline{\lambda_n(j;\nu)}\lambda_n(k;\nu) \quad , \tag{3.7}$$

$$b_\nu(\tau) = a_\nu + V_n^{-\frac{1}{2}}(\tau_\nu\omega_n(\nu))^{-1}\sum_{j=1}^{n}\lambda_n(j;\nu)S^x_{(j)} \quad . \tag{3.8}$$

Let $f_n^o(N;\tau)$ be the specific free energy of $\sum_{\nu\in\mathbb{A}}\omega_n(\nu)a_\nu^*a_\nu + \sum_{\nu\in\mathbb{B}}(1-\tau_\nu)\omega_n(\nu)a_\nu^*a_\nu$, and write $\tilde{f}_n^s(h;N;\tau)$ for that of (3.6). Since the last term in (3.5) is positive, $f_n^o(N;\tau)+\tilde{f}_n^s(h;N;\tau) \leq f_n(h;N)$ by

Bogoljubov's inequality. Thus

$$f_n^o(N) + \tilde{f}_n^s(h;N) - f_n(h;N) \le \{f_n^o(N) - f_n^o(N;\tau)\}$$
$$+ \{\tilde{f}_n^s(h;N) - \tilde{f}_n^s(h;N;\tau)\} \quad . \tag{3.9}$$

Using Bogoljubov's inequality, and the familiar formula for $f_n^o(N;\tau)$

$$f_n^o(N) - f_n^o(N;\tau) \le V_n^{-1} \sum_{\nu\in\mathbb{B}} \tau_\nu \omega_n(\nu) \langle a_\nu^* a_\nu \rangle (N;\tau)$$
$$= - \sum_{\nu\in\mathbb{B}} \tau_\nu \{\partial f_n^o / \partial\tau_\nu\}(N;\tau) = V_n^{-1} \sum_{\nu\in\mathbb{B}} \tau_\nu \omega_n(\nu) (e^{\beta(1-\tau_\nu)\omega_n(\nu)} - 1)^{-1}$$
$$\le (\beta V_n)^{-1} \sum_{\nu\in\mathbb{B}} \tau_\nu (1-\tau_\nu)^{-1} \quad . \tag{3.10}$$

Also using Bogoljubov's inequality and $-\frac{1}{2}1 \le S^x \le \frac{1}{2}1$,

$$\tilde{f}_n^s(h;N) - \tilde{f}_n^s(h;N;\tau) \le V_n^{-2} \sum_{\nu\in\mathbb{B}} \Big\{ (\tau_\nu^{-1} - 1)\omega_n(\nu)^{-1}$$
$$\cdot \mathrm{Re} \sum_{j,k=1}^{n} \overline{\lambda_n(j;\nu)} \lambda_n(k;\nu) \langle S^x_{(j)} S^x_{(k)} \rangle (h;N;\tau) \Big\}$$
$$\le (2V_n)^{-2} \sum_{\nu\in\mathbb{B}} (1-\tau_\nu)\tau_\nu^{-1} \omega_n(\nu)^{-1} \Big[\sum_{j=1}^{n} |\lambda_n(j;\nu)| \Big]^2 \quad . \tag{3.11}$$

Inserting (3.10) and (3.11) into (3.9),

$$\{f_n^o(N) + \tilde{f}_n^s(h;N)\} - f_n(h;N) \le (\beta V_n)^{-1} \sum_{\nu\in\mathbb{B}} \tau_\nu (1-\tau_\nu)^{-1}$$
$$+ (2V_n)^{-2} \sum_{\nu\in\mathbb{B}} (1-\tau_\nu)\tau_\nu^{-1} \omega_n(\nu)^{-1} \Big[\sum_{j=1}^{n} |\lambda_n(j;\nu)| \Big]^2 \quad . \tag{3.12}$$

The infimum of the right hand side of (3.12) with respect to τ is assumed at

$$\tau_\nu = \frac{\beta^{\frac{1}{2}}\ \omega_n(\nu)^{-\frac{1}{2}} \sum_{j=1}^{n} |\lambda_n(j;\nu)|}{2V_n^{\frac{1}{2}} + \beta^{\frac{1}{2}}\ \omega_n(\nu)^{-\frac{1}{2}} \sum_{j=1}^{n} |\lambda_n(j;\nu)|} , \tag{3.13}$$

which lies in (0,1) by virtue of the definition of $\mathbb{B}$. Thus,

$$f_n^o(N)+\tilde{f}_n^s(h;N)-f_n(h;N) \le V_n^{-1}(\beta V_n)^{-\frac{1}{2}} \sum_{\nu\ge 1}^{N} \omega_n(\nu)^{-\frac{1}{2}} \sum_{j=1}^{n} |\lambda_n(j;\nu)| \quad . \tag{3.14}$$

For fixed n, it follows that $f_n^o(N)$, $\tilde{f}_n^s(h;N)$ and $f_n(h;N)$ converge to f_n^o, $\tilde{f}_n^s(h)$ and $f_n(h)$ respectively, as $N \to \infty$, so that the following result is proved.

<u>Lemma</u> <u>2B</u> : $f_n^o + \tilde{f}_n^s(h) - f_n(h) \le V_n^{-1}(\beta V_n)^{-\frac{1}{2}} \sum_{\nu\ge 1} \omega_n(\nu)^{-\frac{1}{2}} \sum_{j=1}^{n} |\lambda_n(j;\nu)|$.

The limit of $\tilde{f}_n^s(h)$ has been recently obtained by Duffield and Pulè [6] in their analysis of the B.C.S. model. Their result, which combines large deviation methods with Berezin-Lieb bounds, is the following

<u>Theorem</u> <u>2</u> (Duffield & Pulè) : *If conditions (C1) and (C2) are satisfied, and there exists a real-valued continous function* h *on* [0,1] *such that*

$$\lim_{n\to\infty} \sup_{j\in\{1,2,\cdots,n\}} |h_j - h(j/n)| = 0 \quad , \tag{C0}$$

then

$$\tilde{f}^s(h) = \lim_{\substack{n\to\infty \\ \rho=\text{const.}}} \tilde{f}_n^s(h) = \rho \inf_{\substack{r,s\in L_{\mathbb{R}}^\infty([0,1]) \\ |s| \le r \le 1}} \Big\{ \int_0^1 \Big[-\beta^{-1} I(r(t)) + \tfrac{1}{2} h(t)s(t)$$

$$- \tfrac{1}{2}|\varepsilon(t)|[r(t)^2 - s(t)^2]^{\frac{1}{2}} \Big] dt - \tfrac{1}{2}\rho \int_0^1 \int_0^1 \Lambda(t,t')s(t)s(t')dtdt' \Big\} \quad .$$

Remark 1: The proofs of ref. 6 apply without change under the slightly stronger assumptions: $h_j=h(j/n)$, $\varepsilon_n(j)=\varepsilon(j/n)$, and $\Lambda_n(j,k)=\Lambda(j/n,k/n)$; but can be adapted to accomodate (C0)-(C2).

$\inf_{x\in\mathbb{R}^n} \hat{f}_n^s(h;x)$ is discussed in Appendix A; one has the following result:

Lemma 3: *Under the assumptions (C0)-(C2),*

$$\lim_{\substack{n\to\infty \\ \rho=\text{const.}}} \inf_{x\in\mathbb{R}^n} \hat{f}_n^s(h;x) = \tilde{f}^s(h) \quad .$$

Proof : Let $M_n=\inf_{x\in\mathbb{R}^n} \hat{f}_n^s(h;x)$; by Lemma A1, setting $s_j=r_j\sin(\vartheta_j)$,

$$M_n = \inf_{|s_j|\le r_j\le 1} \Big\{ V_n^{-1} \sum_{j=1}^{n} \Big\{ -\beta^{-1} I(r_j) - \tfrac{1}{2}|\varepsilon_n(j)|[r_j^2-s_j^2]^{\frac{1}{2}} + \tfrac{1}{2}h_j s_j \Big\}$$

$$- \tfrac{1}{4}V_n^{-2} \sum_{j=1}^{n} \sum_{k=1}^{n} \Lambda_n(j,k)s_j s_k \Big\}\Big\} \quad .$$

Define L_n by replacing $\varepsilon_n(j)$, h_j, and $\Lambda_n(j,k)$ in the above expression for M_n, by $\varepsilon(j/n)$, $h(j/n)$, and $\Lambda(j/n,k/n)$ respectively, where $\varepsilon(\circ)$, $h(\circ)$, and $\Lambda(\circ,\circ)$ are the functions given by conditions (C0)-(C2). As in Theorem 3 of ref. 6, one proves that $L_n \to \tilde{f}^s(h)$ as $n \to \infty$ with ρ=const..Now,

$$|M_n-L_n| \le \sup_{|s_j|\le r_j\le 1} \Big| V_n^{-1} \sum_{j=1}^{n} \Big\{ \tfrac{1}{2}(|\varepsilon(j/n)|-|\varepsilon_n(j)|)[r_j^2-s_j^2]^{\frac{1}{2}}$$

$$+ \tfrac{1}{2}(h_j-h(j/n))s_j \Big\} + \tfrac{1}{4}V_n^{-2} \sum_{j=1}^{n}\sum_{k=1}^{n} (\Lambda(j/n,k/n)-\Lambda_n(j,k))s_j s_k \Big\}\Big|$$

$$\le \tfrac{1}{2}\rho n^{-1} \sum_{j=1}^{n} \Big\{ \big||\varepsilon(j/n)|-|\varepsilon_n(j)|\big| + |h_j-h(j/n)| \Big\}$$

$$+ \tfrac{1}{4}\rho^2 n^{-2} \sum_{j=1}^{n} \sum_{k=1}^{n} |\Lambda(j/n,k/n)-\Lambda_n(j,k)| \quad ,$$

so that, by (C0)-(C2), $M_n - L_n \to 0$ as $n \to \infty$ with ρ=const.∎

<u>Remark 2</u> : One can prove $\lim_{n\to\infty} \{\tilde{f}_n^s(h) - \inf_{x\in\mathbb{R}^n} \hat{f}_n^s(h;x)\}=0$, directly by the "Approximating Hamiltonian Method" using an idea of ref. 1; one has to assume that n^{-1}[number of non-zero eigenvalues of Λ_n] $\to$ 0 as $n \to \infty$; moreover, the positivity of Λ_n is used [11].

The proof of Theorem 1 is obtained combining Lemmas 2A, 2B and 3, and Theorem 2.

One can recover the results of ref. 10 which are valid for the homogeneous case: $\varepsilon_n(j)=\varepsilon_n$, $\lambda_n(j;\nu)=\lambda_n(\nu)$, and $h_j=h$, for all $j=1,2,\cdots,n$ [2]. Condition (C0) is trivially met; conditions (C1) and (C2) demand the existence of real numbers ε, and Λ (≥ 0) such that $\varepsilon_n \to \varepsilon$, and $\langle\lambda_n, \mathfrak{h}_n^{-1}\lambda_n\rangle_{L^2(\mathscr{A}_n)} \to \Lambda$.

<u>Lemma 4</u> : *In the homogeneous case*

$$\tilde{f}^s(h) = -\rho \sup_{0\leq z,u\leq 1} \{\beta^{-1}I(u) + \tfrac{1}{2}|h|u(1-z^2)^{\frac{1}{2}} + \tfrac{1}{2}|\varepsilon|uz + \tfrac{1}{4}\rho\Lambda u^2(1-z^2)\} \ .$$

<u>Proof</u>: By Theorem 2, choosing $r(t)=r$ and $s(t)=s$ a.e.,

$$-\tilde{f}^s(h)/\rho \geq \sup_{|s|\leq r\leq 1} \{\beta^{-1}I(r) - \tfrac{1}{2}hs + \tfrac{1}{2}|\varepsilon|[r^2-s^2]^{\frac{1}{2}} + \tfrac{1}{4}\rho\Lambda s^2\}$$

$$= \sup_{0\leq x,r\leq 1} \{\beta^{-1}I(r) + \tfrac{1}{2}|h|rx + \tfrac{1}{2}|\varepsilon|r[1-x^2]^{\frac{1}{2}} + \tfrac{1}{4}\rho\Lambda r^2x^2\} \quad .$$

For r and s in $L^\infty_{\mathbb{R}}([0,1])$ with $|s|\leq r\leq 1$, (all integrals are over [0,1])

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[2] Condition (C4) is not needed for the results of ref. 10.

$$\int[r(t)^2-s(t)^2]^{\frac{1}{2}}dt = \int[r(t)-s(t)]^{\frac{1}{2}}[r(t)+s(t)]^{\frac{1}{2}}\,dt$$

$$\le \left[\int[r(t)-s(t)]dt\cdot\int[r(t)+s(t)]\,dt\right]^{\frac{1}{2}} = \left[\{\int r(t)dt\}^2-\{\int s(t)dt\}^2\right]^{\frac{1}{2}} ,$$

by the Schwarz inequality; since I is concave,

$$-\tilde{f}^s(h)/\rho \le \sup_{\substack{r,s\in L^\infty_{\mathbb{R}}([0,1])\\ |s|\,\le r\le 1}} \Big\{\beta^{-1}I(\int r(t)dt) - \tfrac{1}{2}h\int s(t)dt + \tfrac{1}{4}\rho\Lambda\{\int s(t)dt\}^2$$

$$+ \tfrac{1}{2}|\varepsilon|\left[\{\int r(t)dt\}^2-\{\int s(t)dt\}^2\right]^{\frac{1}{2}} \Big\}$$

$$= \sup_{|s|\le r\le 1} \{\beta^{-1}I(r) - \tfrac{1}{2}hs + \tfrac{1}{2}|\varepsilon|[r^2-s^2]^{\frac{1}{2}} + \tfrac{1}{4}\rho\Lambda s^2\} \quad .\blacksquare$$

§4. The phase transition

The variational problem determining $\tilde{f}^s(h)$, and thus $f(h)$, is

$$\mathscr{F}(h) = \sup_{\substack{r,s\in L^\infty_{\mathbb{R}}([0,1])\\ |s|\,\le r\le 1}} \Big\{ \int_0^1 \Big[\beta^{-1}I(r(t)) + \tfrac{1}{2}|\varepsilon(t)|[r(t)^2-s(t)^2]^{\frac{1}{2}}$$

$$- \tfrac{1}{2}h(t)s(t)\Big]dt + \tfrac{1}{4}\rho\int_0^1\int_0^1\Lambda(t,t')s(t)s(t')dtdt' \Big\} \quad . \tag{4.1}$$

For $\Lambda(t,t') \ge 0$ (and h=const.) this problem [3], is solved by Duffield and Pulè [(6)]; most of their arguments apply to the case of arbitrary Λ.

Notice that if h=0 and (r,s) is a maximizer for (4.1), then so

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[3] Our kernel need not be positive; it defines a positive operator. $\Lambda(t,t') > 0$ is used in the uniqueness results of ref. 6.

is $(r,-s)$. The function I is concave, with derivative −arctanh. The r-variation can be done as in ref. 6; for $s \in L^{\infty}_{\mathbb{R}}([0,1])$ with $|s| \le 1$, let $r_s:[0,1] \to \mathbb{R}$ be defined (a.e.) to be 1 where $|s|=1$, and otherwise as the *largest* zero in the interval $[|s(t)|,1]$ of the function

$$x \to \tfrac{1}{2}\beta|\varepsilon(t)|x - [x^2-s(t)^2]^{\frac{1}{2}}\operatorname{arctanh}(x) \quad [4] \quad ; \tag{4.2}$$

then, if $\mathcal{B}$ denotes the unit ball of $L^{\infty}_{\mathbb{R}}([0,1])$, one has

$$\mathcal{F}(h) = \sup_{s\in\mathcal{B}} \{\mathcal{V}(s;h)\} \quad , \tag{4.3}$$

where

$$\mathcal{V}(s;h) = \int_0^1 \left[\beta^{-1}I(r_s(t)) + \tfrac{1}{2}|\varepsilon(t)|[r_s(t)^2-s(t)^2]^{\frac{1}{2}} - \tfrac{1}{2}h(t)s(t)\right]dt$$

$$+ \tfrac{1}{4}\rho \int_0^1\int_0^1 \Lambda(t,t')s(t)s(t')dtdt' \quad . \tag{4.4}$$

For h=0, one has inversion symmetry $\mathcal{V}(s;0)=\mathcal{V}(-s;0)$. Let K be the selfadjoint, integral operator on $L^2_{\mathbb{R}}([0,1])$ defined by the kernel Λ; K is compact. Consider the continous function g_β on $[0,1]$ given by

$$g_\beta(t) = \begin{cases} (\beta/2)^{\frac{1}{2}} & , \text{ if } \varepsilon(t)=0 \\ \left[\dfrac{\tanh(\frac{1}{2}\beta|\varepsilon(t)|)}{|\varepsilon(t)|}\right]^{\frac{1}{2}} & , \text{ if } \varepsilon(t)\neq 0 \end{cases} \quad , \tag{4.5}$$

and let G_β be the (bounded, positive) operator on $L^2_{\mathbb{R}}([0,1])$ of multiplication by g_β. Let $U^\rho_\beta=\rho G_\beta K G_\beta$, i.e.

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[4] Notice that $r_0(t)=\tanh(\frac{1}{2}\beta|\varepsilon(t)|)$ a.e., that $r_{-s}=r_s$, and that $r_s=|s|$ on the set where $\varepsilon(t)=0$.

$$\{U^\rho_\beta\psi\}(t) = \rho g_\beta(t)\int_0^1 g_\beta(t')\Lambda(t,t')\psi(t')dt' \quad . \tag{4.6}$$

Define $\Phi^\rho_\beta(s;t)$ (a.e.) by

$$\Phi^\rho_\beta(s;t) = \rho\{Ks\}(t) - \begin{cases} 2\beta^{-1}\mathrm{arctanh}(s(t)) & , \ \varepsilon(t)=0 \\ |\varepsilon(t)|s(t)/[r_s(t)^2-s(t)^2]^{\frac{1}{2}} & , \ \varepsilon(t)\neq 0 \end{cases} \tag{4.7}$$

and notice that $\Phi^\rho_\beta(-s;\circ)=-\Phi^\rho_\beta(s;\circ)$.

The solution of (4.1) for h=0 is obtained from the following two results which will be proved in Appendix B by adjusting the arguments of ref. 6 :

<u>Theorem</u> <u>3</u>: *If* $\|U^\rho_\beta\| \le 1$, *then*

$$\mathcal{f}(0) = \mathcal{V}(0;0) = \beta^{-1}\int_0^1 \log[2\cosh(\tfrac{1}{2}\beta\varepsilon(t))]dt \quad .$$

<u>Theorem</u> <u>4</u>: *If* $\|U^\rho_\beta\| > 1$, *then there exists a non-zero* $s_*\in\mathcal{B}$ *such that* $\mathcal{f}(0)=\mathcal{V}(s_*;0)=\mathcal{V}(-s_*;0)$. s_* *and* $-s_*$ *are solutions of the Euler-Lagrange equation* $\Phi^\rho_\beta(s;\circ)=0$. *Moreover*

$$\mathcal{f}(0) = \mathcal{V}(\pm s_*;0) = \beta^{-1}\int_0^1 \log[2\cosh(\tfrac{1}{2}\beta\{\varepsilon(t)^2+k_\beta(t)^2\}^{\frac{1}{2}})]dt$$

$$- \tfrac{1}{4}\int_0^1 \frac{\tanh(\frac{1}{2}\beta\{\varepsilon(t)^2+k_\beta(t)^2\}^{\frac{1}{2}})}{\{\varepsilon(t)^2+k_\beta(t)^2\}^{\frac{1}{2}}} k_\beta(t)^2 \, dt \quad ,$$

where $k_\beta \neq 0$ *satisfies*

$$k_\beta(t) = \rho\int_0^1 \Lambda(t,t') \frac{\tanh(\frac{1}{2}\beta\{\varepsilon(t')^2+k_\beta(t')^2\}^{\frac{1}{2}})}{\{\varepsilon(t')^2+k_\beta(t')^2\}^{\frac{1}{2}}} k_\beta(t')dt' \quad .$$

__Remark 3__ : Most likely, s_* and $-s_*$ are the *only* non-zero solutions of the Euler-Lagrange equation if K is positive, but I am unable to prove this.

The map $\beta \to \|U^{\rho}_{\beta}\|$ is strictly increasing with $\lim_{\beta \downarrow 0} \|U^{\rho}_{\beta}\| = 0$, so that one can identify a possibly infinite critical reciprocal temperature β_c such that if $\beta < \beta_c$ then $\|U^{\rho}_{\beta}\| < 1$, and if $\beta > \beta_c$ then $\|U^{\rho}_{\beta}\| > 1$. For $\beta \le \beta_c$, $\tilde{f}^s$ - and thus f - is independent of the interaction: the system is thermodynamically equivalent to a non-interacting system of bosons and spins. Qualitatively, the results are identical to those of refs. 9 and 10.

As an illustration, in the homogeneous case, one has

$$\|U^{\rho}_{\beta}\| = \rho\Lambda \begin{cases} \tfrac{1}{2}\beta & \text{, if } \varepsilon=0 \\ \tanh(\tfrac{1}{2}\beta|\varepsilon|)/|\varepsilon| & \text{, if } \varepsilon\neq 0 \end{cases} ,$$

and thus, as in ref. 10,

$$\beta_c = \begin{cases} 2\operatorname{arctanh}(|\varepsilon|/\rho\Lambda)/|\varepsilon| & \text{, if } \varepsilon\neq 0 \text{ and } |\varepsilon| < \rho\Lambda \\ +\infty & \text{, if } \varepsilon\neq 0 \text{ and } |\varepsilon| \ge \rho\Lambda \\ 2/(\rho\Lambda) & \text{, if } \varepsilon=0 \end{cases} .$$

Finally, one can proceed as in ref. 6, to obtain the thermodynamic limit of the equilibrium expectation of the average spin-polarization in x-direction when $h(t)=\hbar$ (by symmetry this limit is zero for $\hbar=0$); and then consider the limit $\hbar \to 0$. The result is qualitatively the same as that for the homogeneous case [(10)], namely: the limit is zero for $\beta \le \beta_c$, and *not* zero if $\beta > \beta_c$ with different sign depending on whether $\hbar\uparrow 0$ or $\hbar\downarrow 0$.

__Appendix A__: Discussion of $\inf_{x\in\mathbb{R}^n} \tilde{f}^s_n(h;x)$

__Lemma A1__ : *Let* I *on* [0,1] *be defined as in Theorem 1. Then,*

$$\inf_{x\in\mathbb{R}^n} \hat{f}_n^s(h;x) = \inf_{\substack{r_j\in[0,1] \\ \vartheta_j\in[0,2\pi]}} \Big\{ V_n^{-1} \sum_{j=1}^{n} \Big\{ -\beta^{-1} I(r_j) + \tfrac{1}{2}\varepsilon_n(j) r_j \cos(\vartheta_j)$$

$$+ \tfrac{1}{2} h_j r_j \sin(\vartheta_j) - \tfrac{1}{4} V_n^{-1} \sum_{k=1}^{n} \Lambda_n(j,k) r_j r_k \sin(\vartheta_j)\sin(\vartheta_k) \Big\}\Big\}$$

$$= \inf_{\substack{r_j\in[0,1] \\ \vartheta_j\in[-\frac{1}{2}\pi,\frac{1}{2}\pi]}} \Big\{ V_n^{-1} \sum_{j=1}^{n} \Big\{ -\beta^{-1} I(r_j) - \tfrac{1}{2}|\varepsilon_n(j)| r_j \cos(\vartheta_j)$$

$$+ \tfrac{1}{2} h_j r_j \sin(\vartheta_j) - \tfrac{1}{4} V_n^{-1} \sum_{k=1}^{n} \Lambda_n(j,k) r_j r_k \sin(\vartheta_j)\sin(\vartheta_k) \Big\}\Big\} \quad .$$

<u>Proof</u> : One verifies that for a and b real,

$$\inf_{\substack{r\in[0,1] \\ y^2+z^2=1}} \{-\beta^{-1} I(r) + \tfrac{1}{2}\, arz + \tfrac{1}{2} bry\} = -\beta^{-1}\log(2\cosh(\tfrac{1}{2}\beta[a^2+b^2]^{\frac{1}{2}})) \quad .$$

Thus, by Lemma 1,

$$\hat{f}_n^s(h;x) = V_n^{-1} \inf_{\substack{r_j\in[0,1] \\ z_j^2+y_j^2=1}} \sum_{j=1}^{n} \Big\{ -\beta^{-1} I(r_j) + \tfrac{1}{2}\varepsilon_n(j) r_j z_j$$

$$+ \tfrac{1}{2} r_j y_j \Big[h_j - 2\sum_{k=1}^{n} \Lambda_n(j,k) x_k \Big] \Big\} + x\Lambda_n x \quad .$$

The variation over $x \in \mathbb{R}^n$ can be done explicitely (for this, it is convenient to diagonalize Λ_n); it follows that

$$\inf_{x\in\mathbb{R}^n} \hat{f}_n^s(h;x) = V_n^{-1} \inf_{\substack{r_j\in[0,1] \\ z_j^2+y_j^2=1}} \sum_{j=1}^{n} \Big\{ -\beta^{-1} I(r_j) + \tfrac{1}{2}\varepsilon_n(j) r_j z_j$$

$$+ \tfrac{1}{2}h_j r_j y_j - \tfrac{1}{4}V_n^{-1} \sum_{k=1}^{n} r_j r_k y_j y_k \Lambda_n(j,k)\Big\} \quad ,$$

which proves the first claim upon setting $z_j = \cos(\vartheta_j)$, $\vartheta_j \in [0,2\pi]$. The second claim is obvious.■

<u>Appendix</u> <u>B</u> : Solution of the variational problem following Duffield and Pulè [6].

Write $\mathcal{S}$ for $\mathcal{S}(0)$, and $\mathcal{V}(s)$ for $\mathcal{V}(s;0)$.

<u>Proof</u> <u>of</u> <u>Theorem</u> <u>3</u> : This is a minor adjustment of the corresponding result of ref. 6, to accomodate the fact that our variation is over $\mathcal{B}$ and not its positive part. Let A be the support of ε. For arbitrary $s \in \mathcal{B}$ and $0 < p < 1$, put $F(p) = \mathcal{V}(ps)$. F is differentiable with derivative (integrals with unspecified domain are over [0,1])

$$F'(p) = \tfrac{1}{2}p\rho \iint \Lambda(t,t')s(t)s(t')dtdt'$$

$$- \tfrac{1}{2}p \int_A |\varepsilon(t)|s(t)^2[r_{ps}(t)^2 - p^2 s(t)^2]^{-\frac{1}{2}}dt$$

$$-\beta^{-1}\int_{A^c} \operatorname{arctanh}(p|s(t)|)|s(t)|dt \quad .$$

Using the inequalities

$$|s(t)|\operatorname{arctanh}(p|s(t)|) \geq p\, s(t)^2 \quad ,$$

$$[r_s(t)^2 - s(t)^2]^{\frac{1}{2}} \leq \tanh(\tfrac{1}{2}\beta|\varepsilon(t)|) \quad ,$$

one obtains $F'(p) \leq \tfrac{1}{2}p\langle \bar{s}, (U_\beta^\rho - 1)\bar{s}\rangle_{L^2_{\mathbb{R}}([0,1])}$, where $\bar{s}(t) = s(t)/g_\beta(t)$. The assumption $\|U_\beta^\rho\| \leq 1$ implies $F'(p) \leq 0$, so that $\mathcal{V}(ps) \leq \mathcal{V}(0)$, and by continuity $\mathcal{V}(s) \leq \mathcal{V}(0)$. $\mathcal{V}(0)$ can be computed using $r_0(t) = \tanh(\tfrac{1}{2}\beta|\varepsilon(t)|)$.■

The proof of Theorem 4 is broken up into a series of lemmas all of which have their origins in ref. 6.

Lemma B1 : *There exists* $s \in \mathcal{B}$ *such that* $\mathcal{S}(h)=\mathcal{V}(s;h)$.

Proof : See Theorem 5 of ref. 6.∎

Lemma B2 : *If* $\|U_\beta^\rho\| > 1$ *then* $\mathcal{S} > \mathcal{V}(0)$.

Proof : Let $s \in \mathcal{B}$ with $\mathcal{V}(s)=\mathcal{S}$. Since U_β^ρ is compact, $\|U_\beta^\rho\|$ is an eigenvalue; let ξ be a corresponding eigenvector. Define $\xi_n \in L^\infty_{\mathbb{R}}([0,1])$ by

$$\xi_n(t) = \begin{cases} \xi(t) & , \text{ if } |\xi(t)| \le n \\ 0 & , \text{ otherwise} \end{cases} \quad , \text{a.e.} \quad .$$

It follows that $\langle\xi_n,(U_\beta^\rho-1)\xi_n\rangle_{L^2_{\mathbb{R}}([0,1])} \to \|U_\beta^\rho\|-1$ (>0 !) as $n \to \infty$. Choose m such that $\langle\xi_m,(U_\beta^\rho-1)\xi_m\rangle_{L^2_{\mathbb{R}}([0,1])} > 0$, and let $\hat{s}=\xi_m g_\beta$. The proof then proceeds as in Lemma 3 of ref. 6 ∎

Lemma B3 : *If* $s \in \mathcal{B}$ *and* $\mathcal{S} = \mathcal{V}(s)$, *then* $\{t\in[0,1]:|s(t)|=1\}$ *has zero measure.*

Proof : Proceed as in the proof of Lemma 2 of ref. 6, with the set $\{t\in[0,1]:|s(t)|=1\}$.∎

Lemma B4 : *If* $s \in \mathcal{B}$, *and* $\mathcal{S} = \mathcal{V}(s)$, *then* $\Phi_\beta^\rho(s;\circ)=0$.

Proof : This is an adaptation of the proof of Theorem 6 of ref. 6. Let $0 < \delta < 1$, and take $\xi \in L^\infty_{\mathbb{R}}([0,1])$ with essential support contained in $A_\delta\equiv\{t\in[0,1]:|s(t)|<1-\delta\}$. For $|p|$ sufficently small, $s_p=s[1+p\xi]$ lies in $\mathcal{B}$. Let $F(t)=\mathcal{V}(s_p)$. Taking the derivative at $p=0$, one obtains

$$\tfrac{1}{2}\int_{A_\delta} \xi(t)s(t)\Phi_\beta^\rho(s;t)dt = 0 \quad . \qquad (*)$$

Now take $\xi = s\Phi^{\rho}_{\beta}(s;\circ)$ on A_{δ}, and $\xi=0$ on A^{c}_{δ} ; (*) implies that $s\Phi(s;\circ)=0$ on A_{δ}. Since δ was arbitrary, Lemma B3 implies that $s\Phi^{\rho}_{\beta}(s;\circ)=0$. Thus, $\Phi^{\rho}_{\beta}(s:\circ)=0$ on B, the essential support of s; but by the definition of $\Phi^{\rho}_{\beta}(s;\circ)$, $\Phi^{\rho}_{\beta}(s;\circ)=0$ on B^{c}.■

The first part of Theorem 4 follows from Lemmas B2-B4; the rest of the claim follows as in ref. 6.

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